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Nikolov, Nikolai Georgiev; Cross, Kevin P.; Quigley, Patrick; Dybdahl, Marianne; Reffstrup, Trine Klein; Abildgaard Rosenberg, Sine; Wedebye, Eva Bay

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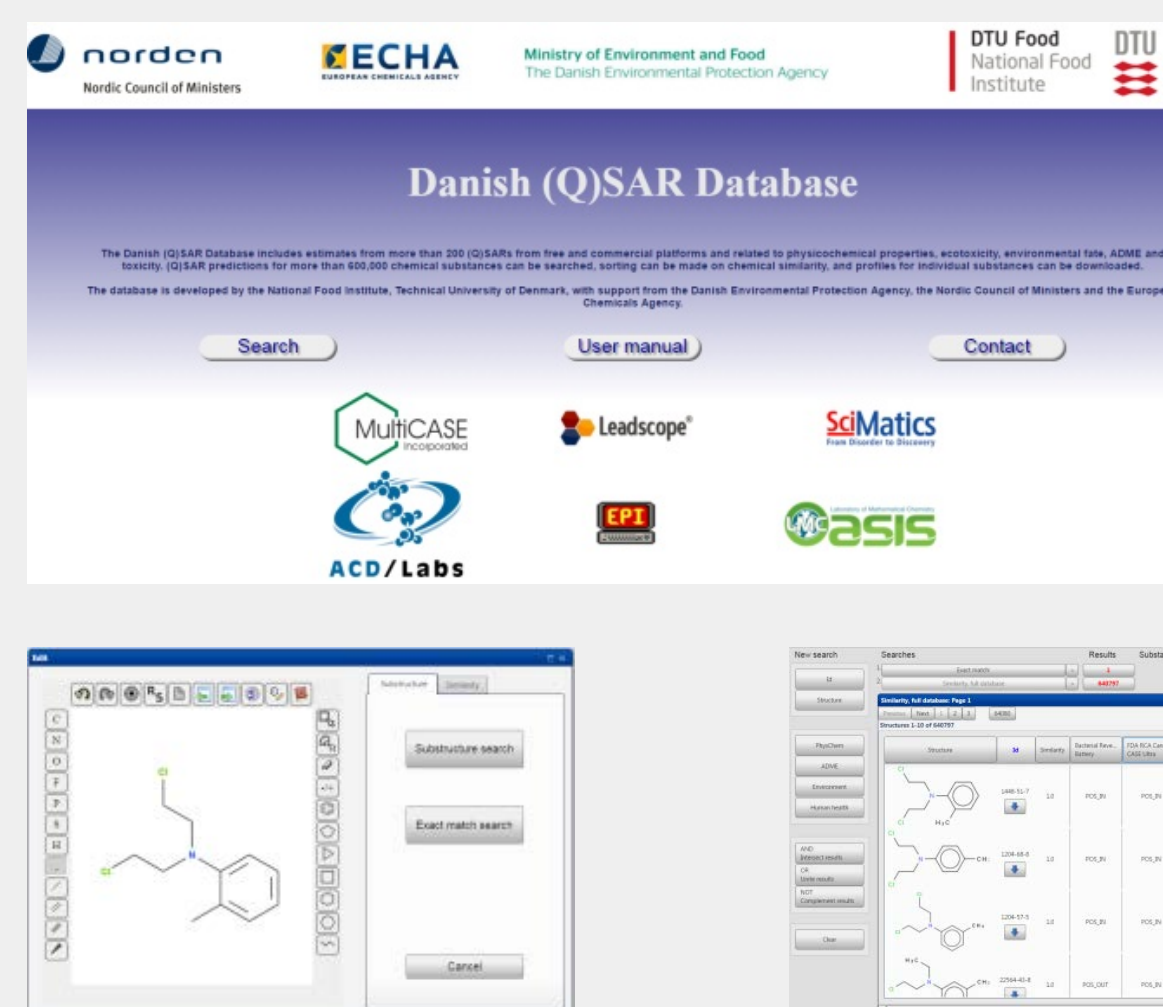
Danish (Q)SAR Models: A free online DTU QSAR predictor powered by Leadscope

Nikolai G. Nikolov¹, Kevin P. Cross², Patrick Quigley², Marianne Dybdahl¹, Trine K. Refstrup¹, Sine A. Rosenberg¹, Eva B. Wedebye¹
¹Technical University of Denmark, ²Leadscope Inc.

The QSAR team at the Technical University of Denmark, National Food Institute, has recently published a completely rebuilt version of the Danish (Q)SAR Database (<http://qsar.food.dtu.dk>) with pre-generated predictions from a large number of QSAR models for over 600,000 chemical structures. A selection of more than 20 of these QSAR models of diverse endpoints encompassing acute toxicity, metabolism, endocrine activity, genotoxicity and sensitization have been implemented in a real-time online predictive system. The system generates predictions on the fly for user-submitted structures and uses Leadscope Enterprise software as a back-end to the web server. All models have undergone robust cross-validation, and documentation in the international QMRF format is available from the website.

Danish (Q)SAR Database: Predictions from >200 (Q)SAR models pre-calculated for >600,000 substances

- DTU-developed, commercial and free models
- 72,000 EU REACH chemical substances and 372,000 NIH MLSMR
- Battery predictions: 3 QSAR approaches for the same training set
- Database, client and server software developed by DTU Food



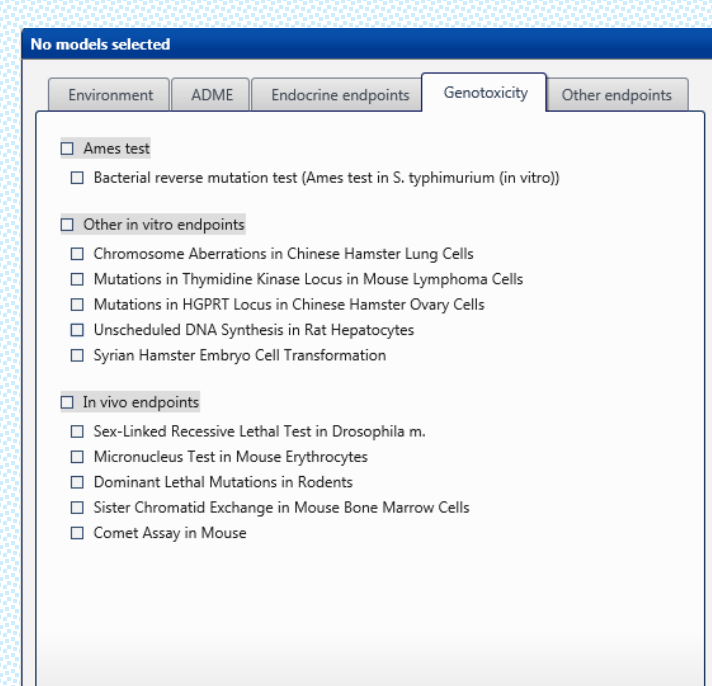
- Single substance look-up by ID or structure: profiling
- Screening across all QSAR-predicted and experimental properties and structures
- Sort on chemical similarity for read-across purposes
- Free for everyone to use

Danish (Q)SAR Models: Online prediction generation from >20 of the Danish (Q)SAR Database models

The Leadscope versions of selected models are made available for real-time prediction. The client/server software is developed by DTU Food and Leadscope Enterprise server is used as a back-end.

Included models

- Acute aquatic toxicity (Fish, Daphnia, Algae)
- Cytochrome P450 substrates (2C9, 2D6)
- Endocrine (ER binding/agonism, AR antagonism, *in vitro*)
- Genotoxicity *in vitro* (Ames test in Salmonella t., Chromosome aberrations in CHL, Mutations in Mouse Lymphoma, Mutations in HGPRT Locus in CHO, Unscheduled DNA Synthesis in Rat hepatocyte, SHE Cell Transformation), *in vivo* (Drosophila m. SLRL, Mouse Micronuclei, Rodent Dominant Lethal, Mouse Sister Chromatid Exchange, Mouse Comet Assay)
- Acute toxicity (Maximum recommended daily dose, human)
- Skin irritation (Severe skin irritation in Rabbit)
- Respiratory sensitization (human)
- Cardiotoxicity (hERG blocking, *in vitro*)

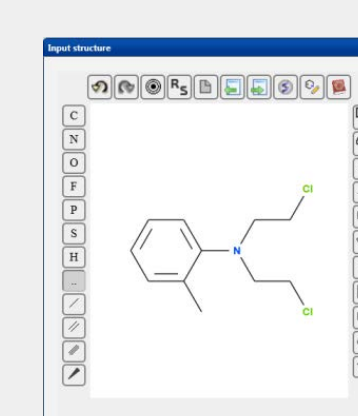


On-the-fly prediction generation:

- Same prediction and domain call as in the Danish (Q)SAR Database
- Positive prediction probability
- Detailed report with structural alerts and training set analogs

Chemical structure input

Draw, enter SMILES,
MOL/SDF or look up by name:

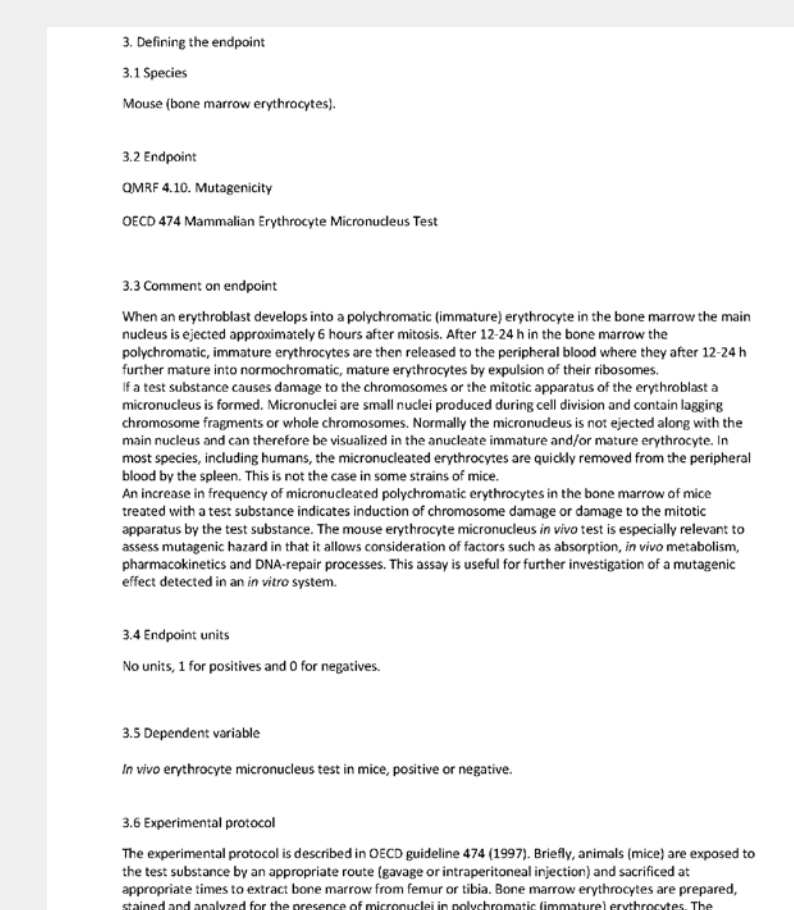


Predictions and reports download

QSAR Results					
Model	Probability	Prediction	Report		
ER alpha binding (human in vitro), all	0.155	NEG_IN			
ER alpha activation (human in vitro)	0.0186	NEG_IN			
Androgen receptor antagonism (human in vitro)	0.138	NEG_OUT			
Unscheduled DNA Synthesis in Rat Hepatocytes	0.308	NEG_OUT			
Micronucleus Test in Mouse Erythrocytes	0.96	POS_IN			
Dominant Lethal Mutations in Rodents	0.979	POS_IN			
Maximum recommended daily dose (MRDD) in Humans	0.51	POS_OUT			

All Predictions					
Positive Predictions		Negative Predictions		Analog Structures in DK_DB_DNC_1_Model v1	
Structure	Probability	Structure	Probability	Structure	Probability
	0.155		0.138		0.155
	0.0186		0.138		0.138
	0.138		0.138		0.138
	0.308		0.308		0.308
	0.96		0.96		0.96
	0.979		0.979		0.979
	0.51		0.51		0.51

QMRF reports



Works in a browser,
no need to install
programs, no
plugins or add-ons
required. All major
browsers and
operating systems
are supported.